

## Mass defect and chemical bond.

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When a chemical bond is formed, a certain energy is always released into the surrounding space. Consequently, a mass defect must also inevitably arise, since the binding energy is the difference between the energy of individual atoms (infinitely distant from each other) and the energy of atoms bound by a chemical bond.

Let atoms a and b form a diatomic molecule a-b. Given the Einstein formula, it is easy to determine the mass defect from the chemical bond energy:

$$E(a-b) = \Delta m * c^2$$

$$\Delta m = E(a-b) / c^2$$

where  $E(a-b)$  is the energy of the chemical bond between atoms a and b,

$\Delta m$  is the mass defect of a given chemical bond,  $c$  is the speed of light in vacuum.

It should be recalled that theoretically strictly the sum of the masses of the objects that make up the system is not equal to the mass of the system. Therefore, when theoretically determining the mass defect of a chemical bond, one cannot compare the mass of a diatomic molecule and the sum of the masses of nuclei and electrons.

In an isolated physical system, only energy and momentum are conserved, in accordance with Noether's theorem. Moreover, energy and momentum are related by the Einstein formula, from which it is already possible to determine the mass of the system:

$$E^2 = (p * c)^2 + (m * c^2)^2$$

“...Historically, the principle of the equivalence of mass and energy was first formulated in its final form when Albert Einstein built the special theory of relativity.

He showed that for a freely moving particle, as well as a free body and, in general, any closed system of particles, the following relations hold:

$$E^2 = (p * c)^2 + (m * c^2)^2$$

$$p = (E * v) / c^2$$

where  $E$ ,  $p$ ,  $v$ ,  $m$  are energy, momentum, velocity and invariant mass of a system or particle, respectively,  $c$  is the speed of light in vacuum.

From these expressions it can be seen that in relativistic mechanics, even when the velocity and momentum of a body (a massive object) vanish, its energy does not vanish, remaining equal to a certain value determined by the mass of the body:

$$E = m * c^2$$

This quantity is called rest energy, and this expression establishes the equivalence of the body mass to this energy. Based on this fact, Einstein concluded that body mass is one of the forms of energy and that thereby the laws of conservation of mass and energy are combined into one conservation law..." [1].

The law of conservation of mass (the mass of a closed physical system is equal to the sum of the masses of its components) used in chemistry is an approximation. This is very clearly seen in the example of a proton and a neutron: a proton and a neutron consist of three quarks, the sum of the masses of these quarks is only 1 % of the actual mass of the proton and 1.3 % of the real mass of the neutron.

Understanding that a certain mass defect exists during the formation of a chemical bond is very important, since it is the essence of the physical justification of a chemical bond.

For further reasoning, we first consider the Bohr model of the atom, then the molecular hydrogen ion and the hydrogen molecule.

A hydrogen atom is formed from a proton and an electron, and the binding energy, that is, the ionization energy is 13.6 eV [2].

According to Bohr, an electron in a hydrogen atom moves in orbit at a speed  $v = 2.187691 * 10^6$  m/s.

Moreover,  $v$  is equal to:

$$v = c * \alpha = 2.187691264 * 10^6$$
 m/s

where  $v$  is the speed of an electron in the Bohr orbit,

$c$  is the speed of light in vacuum,

$\alpha$  is the fine structure constant,  $\alpha = 7.2973525693 * 10^{-3}$ .

According to the theory of relativity, the mass of a moving electron will increase, and will be  $m = 9.109626 * 10^{-31}$  kg.

$$m = m_0 / (1 - v^2/c^2)^{0.5}$$

$m_0$  is the rest mass of an electron,  $m_0 = 9.1093837 * 10^{-31}$  kg.

$$v = 2.187691264 * 10^6 \text{ m/s}$$

$$m = m_0 / (1 - v^2/c^2)^{0.5} = 9.10962625 * 10^{-31} \text{ kg}$$

We especially note that the mass defect in the formation of a hydrogen atom is exactly equal to the relativistic addition of the electron mass:

$$\Delta m = m - m_0 = 2.425529 * 10^{-35} \text{ kg}$$

Using the mass defect for an electron, it is easy to obtain the ionization energy of a hydrogen atom.

$$E = \Delta m * c^2 = 2.1799567 * 10^{-18} \text{ J} = 13.606 \text{ eV}$$

Thus, the binding energy in the hydrogen atom is formed due to the mass defect (electron), and the relativistic mass of the electron decreases to the rest mass of the electron.

Reducing the mass of an electron to a rest mass is very important, as it is a guarantee of the non-stop motion of an electron: when an electron slows down or stops, its mass, according to Einstein's STR, must decrease, and this is impossible (the mass of an electron is already a rest mass). Therefore, in the Bohr orbit, the electron will always move, that is, there will be no stopping, collisions, slowing down, etc.

For a similar reason, a photon can only move at the speed of light - the rest mass of a photon is zero, therefore, a decrease in mass is impossible (when the speed decreases or stops), which means that a photon can only move at the speed of light.

Due to the effects of the theory of relativity, the Bohr radius and standing wave length will also decrease. Let's correct their value.

The Bohr radius is:

$$r_0 = 0.52917720859 * 10^{-10} \text{ m} \approx 0.529177 \text{ \AA}$$

We take into account the relativistic decrease and obtain a more accurate value of the Bohr radius:

$$r = r_0 * (1 - v^2/c^2)^{0.5} = 0.52916311871 * 10^{-10} \text{ m} \approx 0.529163 \text{ \AA}$$

Let us calculate the length of the standing wave in the Bohr orbit:

$$\lambda_0 = 2 * \pi * r_0 = 3.32491846191 * 10^{-10} \text{ m} \approx 3.324919 \text{ \AA}$$

Now we take into account the relativistic reduction for a standing wave:

$$\lambda = \lambda_0 * (1 - v^2/c^2)^{0.5} = 2 * \pi * r = 3.32482993263 * 10^{-10} \text{ m} \approx 3.324830 \text{ \AA}$$

Next, consider the hydrogen molecule.

The dissociation energy of a hydrogen molecule is 4.477 eV. This means that when two hydrogen atoms distant to infinity approach each other (at an internuclear distance of 0.7416 Å), a hydrogen molecule is formed, and a binding energy of 4.477 eV is released [3].

Earlier it was shown that when an electron moves in a Bohr orbit, the speed of an electron cannot be fundamentally changed. Therefore, it is logical to assume that when a hydrogen molecule is formed, the speed of an electron will remain the same (like that of a hydrogen atom). Therefore, the question arises: where does the additional energy come from, which is released during the formation of a hydrogen molecule?

The answer to this question is given by Einstein's STR, or rather the concept of "longitudinal" and "transverse" mass [4].

The electron in the hydrogen atom moves in a circle, that is, the linear speed of the electron is always perpendicular to the acceleration. Therefore, the relativistic increase in the mass of an electron in a Bohr orbit is an increase in the "transverse mass" ( $v \uparrow, a \rightarrow$ ).

$$m(v \uparrow, a \rightarrow) = m_0 / (1 - v^2/c^2)^{0.5}$$

The movement of chemical bond electrons will no longer be a simple movement along a circular orbit (as it was in the hydrogen atom), it will be a much more complex movement along an ellipse, a straight line, etc. In any case, for some time the speed and acceleration of the electron will be directed along the same line, and therefore, in relativistic effects, one must also take into account the "longitudinal mass" ( $v \rightarrow, a \rightarrow$ ).

$$m(v \rightarrow, a \rightarrow) = m_0 / (1 - v^2/c^2)^{1.5}$$

Since the "longitudinal mass" is greater than the "transverse" one (at a given speed of movement), then during the formation of a chemical bond (from atoms), additional binding energy will be released, which is due to the defect in the "longitudinal mass" of the electron. It is clear that the speed will not change in this case, but only the direction of motion of the electron relative to the force will change.

A chemical bond can also be viewed as a linear harmonic oscillator, that is, when a particle performs one-dimensional oscillations near the equilibrium position (the center of the chemical bond). In this case, there will also be an increase in the "longitudinal mass", since the particle will oscillate between the nuclei of atoms.

Let us demonstrate what was said above using the example of the molecular hydrogen ion ( $\text{H}_2^+$ ).

The dissociation energy of a molecular hydrogen ion is 2.648 eV [3].

$$E = 2.648 \text{ eV} = 4.24256371624 * 10^{-19} \text{ J} \approx 4.242564 * 10^{-19} \text{ J}$$

The internuclear distance in  $\text{H}_2^+$  is 1.06 Å.

Let us assume that an electron in a molecular hydrogen ion performs only one-dimensional motion when its velocity and acceleration are directed along the same line. Then, from the “longitudinal mass” defect, we can easily obtain the maximum amount of energy that can theoretically be released during the formation of  $\text{H}_2^+$ .

It is clear that in reality the released energy will be less, since when the electron moves, not only the “longitudinal mass”, but also the “transverse mass” increase. Therefore, the total energy balance from the mass defect (longitudinal and transverse) will be less. A similar decrease will be observed in all chemical bonds, since the electrons of a chemical bond are involved not only in the formation of a bond, but also “serve” the octets of individual atoms. Let us present the calculations.

Let us assume that the speed of an electron in  $\text{H}_2^+$  will be equal to the speed of an electron in a Bohr orbit.

$$v = 2.187691264 * 10^6 \text{ m/s}$$

Then the “longitudinal mass” of the electron is calculated by the formula:

$$m = m_0 / (1 - v^2/c^2)^{1.5} = 9.11011137926 * 10^{-31} \text{ kg} \approx 9.1101114 * 10^{-31} \text{ kg}$$

Hence it is easy to obtain a defect in the “longitudinal mass” of the electron.

$$\Delta m = m - m_0 = 7.2767925 * 10^{-35} \text{ kg}$$

Using the mass defect, we calculate theoretically the maximum energy.

$$E_{\text{max}} = \Delta m * c^2 = 6.5400549 * 10^{-18} \text{ J}$$

Note that the obtained value of the maximum energy ( $E_{\text{max}}$ ) is greater than the sum of the repulsion energy of protons and the dissociation energy, since when an electron moves in a molecular hydrogen ion, its speed and acceleration will sometimes be perpendicular, and therefore the mass defect will sometimes be determined by the “transverse mass”.

The energy that the molecular hydrogen ion “receives” from the mass defect will be spent on overcoming the protons repulsion energy (distance 1.06 Å), and the remainder of this energy will be released and will be the dissociation energy of the molecular hydrogen ion.

The repulsion energy of protons in a molecular hydrogen ion is:

$$E = (k * e^2) / r$$

where  $k$  is the Coulomb constant,  $e$  is the electron charge,

$r$  is the distance between protons, that is, 1.06 Å.

$$E_{p-p} = (k * e^2) / r = 2.176488 * 10^{-18} \text{ J}$$

Recall that the dissociation energy of a molecular hydrogen ion is:

$$E_d = 4.242564 * 10^{-19} \text{ J}$$

Let us calculate the sum of the proton repulsion energy and the dissociation energy.

$$E_s = E_{p-p} + E_d = 2.6007446 * 10^{-18} \text{ J}$$

Let's calculate the value of  $E_{max} / E_s$ .

$$E_{max} / E_s = 6.5400549 * 10^{-18} \text{ J} / 2.6007446 * 10^{-18} \text{ J}$$

$$E_{max} / E_s = 2.514686 \approx 2.515$$

As we can see, the maximum energy is 2.5 times greater than the obtained sum of energies, which was to be expected based on our assumptions.

We will observe a similar situation in the hydrogen molecule. Let's demonstrate this.

Let us assume that two electrons in a hydrogen molecule perform only certain one-dimensional motions when their velocity and acceleration are directed along the same line (only the “longitudinal mass” increases). As usual, we assume that the speed of chemical bond electrons is equal to the speed of an electron in the first Bohr orbit. Therefore, the maximum energy calculated from the mass defect for one electron will be equal to the maximum energy calculated for the molecular hydrogen ion.

Recall that the “longitudinal mass” defect for one electron in  $H_2^+$  is equal to:

$$\Delta m = m - m_0 = 7.2767925 * 10^{-35} \text{ kg}$$

Theoretically, the maximum energy is (1 electron):

$$E_{\max} = \Delta m * c^2 = 6.5400549 * 10^{-18} \text{ J}$$

The chemical bond of a hydrogen molecule consists of two electrons, therefore, the maximum energy that can be “obtained” from the electron mass defect will be twice as much.

$$E_{\max} (\text{H-H}) = 2 * \Delta m * c^2 = 2 * 6.5400549 * 10^{-18} \text{ J} = 1.30801098 * 10^{-17} \text{ J}$$

$$E_{\max} (\text{H-H}) \approx 1.308011 * 10^{-17} \text{ J}$$

Since a hydrogen molecule consists of two protons (distance 0.7416 Å) and two electrons (form a chemical bond), the total energy balance in the formation of a molecule from protons and electrons can be easily calculated. It will be equal to twice the ionization potential of the hydrogen atom plus the dissociation energy of the hydrogen molecule.

The ionization potential of the hydrogen atom is 13.6 eV.

$$E_i = 13.6 \text{ eV} = 2.17896022 * 10^{-18} \text{ J}$$

The dissociation energy of a hydrogen molecule is 4.477 eV.

$$E(\text{H-H}) = 4.477 \text{ eV} = 7.17294477 * 10^{-19} \text{ J}$$

Let us calculate the total energy balance.

$$E(\text{bal}) = 2 * E_i + E(\text{H-H}) = 2 * 13.6 \text{ eV} + 4.477 \text{ eV} = 2.89625469 * 10^{-18} \text{ J}$$

Let's compare the obtained balance with the maximum energy.

$$E_{\max} (\text{H-H}) / E(\text{bal}) = 1.30801098 * 10^{-17} \text{ J} / 2.89625469 * 10^{-18} \text{ J}$$

$$E_{\max} (\text{H-H}) / E(\text{bal}) = 4.5162153 \approx 4.516$$

That is, the maximum possible energy in a hydrogen molecule (from the mass defect) is 4.5 times greater than the actual energy balance calculated by us. As in the case of the molecular hydrogen ion, the actual balance in the hydrogen molecule is less than the theoretical maximum, since electrons move part of the time when their speed and acceleration are perpendicular. That is, in the mass defect, it is necessary to take into account not only the “longitudinal mass”, but also the “transverse mass”.

The energy “received” from the real mass defect  $E(\text{bal})$  will be spent on overcoming the repulsion energy of protons in the hydrogen molecule, on the energy of repulsion of electrons, and the rest of the energy is the dissociation energy of the molecule (H-H). Let us calculate the electron repulsion energy.

First, let's calculate the repulsion energy of protons in a hydrogen molecule, which is (distance 0.7416 Å):

$$E_{\text{p-p}} = (k * e^2) / r = 3.11094598 * 10^{-18} \text{ J}$$

Given the overall energy balance and dissociation energy of the molecule, it is easy to calculate the repulsion energy of electrons in the hydrogen molecule.

$$E_{\text{e-e}} = E(\text{bal}) - E_{\text{p-p}} - E(\text{H-H})$$

$$E_{\text{e-e}} = 2.89625469 * 10^{-18} \text{ J} - 3.11094598 * 10^{-18} \text{ J} - 7.17294477 * 10^{-19} \text{ J}$$

$$E_{\text{e-e}} = -0.931985767 * 10^{-18} \text{ J}$$

Thus, we have found that the total energy balance of the molecule is not enough to compensate for the electron repulsion energy. This means that there must be a correct physical process of interaction of electrons, in which energy sufficient to neutralize the repulsion between these electrons will be released.

Suppose that two chemical bond electrons with opposite spins move in parallel and in concert (along the chemical bond), that is, they behave like a Cooper pair of electrons. Then, we will get two parallel currents, which will be attracted to each other according to Ampère's law. We know the interaction energy, so we can easily calculate the distance between the interacting electrons (the distance between the currents). Let's give a calculation.

According to Ampere's law, two conductors of length  $L$ , with currents  $I(1)$  and  $I(2)$ , and the distance between the conductors  $r$ , will be attracted to each other with a force equal to [5]:

$$F = (\mu_0 * 2 * I(1) * I(2) * L) / (4 * \pi * r)$$

where  $\mu_0$  is the magnetic constant,  $\mu_0 = 1.25663706212 * 10^{-6} \text{ H/A}^2$

By definition, the current strength is the ratio of the amount of charge  $\Delta q$  passed over a certain time  $\Delta t$  to the value of this time interval.

$$I = \Delta q / \Delta t$$

Naturally,  $\Delta q$  is the charge of an electron, which during the time  $\Delta t$  at a speed  $v$  will pass the length of the chemical bond. We know the speed of the electron (this is the speed on the Bohr orbit), the length of the chemical bond is known, we calculate  $\Delta t$ .

$$\Delta t = L / v = 0.7416 * 10^{-10} \text{ m} / 2.187691264 * 10^6 \text{ m/s}$$

$$\Delta t = 3.38987504 * 10^{-17} \text{ s}$$

Knowing  $\Delta t$ , we can calculate the current strength:

$$I = \Delta q / \Delta t = e / \Delta t = 1.60217663 * 10^{-19} \text{ C} / 3.38987504 * 10^{-17} \text{ s}$$

$$I = 4.72635897 * 10^{-3} \text{ A}$$

Considering that our currents are the same, and the Ampère force will act along the entire length of the chemical bond ( $L$ ), we can assume that the interaction energy will be equal to:

$$E = F * L = (\mu_0 * 2 * I^2 * L^2) / (4 * \pi * r)$$

From here we get the distance between the electrons in the hydrogen molecule:

$$r = (\mu_0 * 2 * I^2 * L^2) / (4 * \pi * E) = 2.63641373 * 10^{-14} \text{ m}$$

We especially note that the distance between electrons is 92 times less than the Compton wavelength of an electron:

$$\lambda_{c.e.} / r = 2.4263086 * 10^{-12} \text{ m} / 2.63641373 * 10^{-14} \text{ m} = 92.031$$

This is a very important result, which once again confirmed that chemical bond electrons can no longer be considered as point particles, and therefore, the Pauli principle is not applicable to such electrons (there are no separate electrons, but there is a “boiling mass” of real electrons and virtual positrons and electrons).

Recall that an electron in a region with linear dimensions smaller than the Compton wavelength can no longer be considered as a “point object”, since the electron spends part of its time in the “electron + pair (positron + electron)” state. According to the Heisenberg uncertainty principle in this area, we have a quantum mechanical uncertainty of momentum and energy sufficient for the creation of virtual electron-positron pairs.

“...This approach makes it possible to explain how, in the case of many-electron chemical bonds (two-electron, three-electron, etc.), repulsion between electrons is overcome: since the chemical bond is actually a “boiling mass” of electrons and positrons, virtual positrons “help” overcome the repulsion between electrons. This approach assumes that the chemical bond is in fact a closed spatial bag (a potential well in the energy sense), in which “boiling” of real electrons and also virtual positrons and electrons occurs, and the “volume” of this potential bag is actually a “volume” of chemical bond and also the spatial measure of the quantum-mechanical uncertainty in the position of the electron.

Strictly speaking, with such a consideration, the electron no longer has a certain energy, momentum, coordinates, and is no longer a “point particle”, but actually takes up the “whole volume” of chemical bonding. It can be argued that in the chemical bond a single electron is depersonalized and loses its individuality, in fact it does not exist, but there is a “boiling mass” of real electrons and virtual positrons and electrons that by fluctuate change each other....” [6].

The calculated distance between electrons ( $2.636 * 10^{-14}$  m) in a hydrogen molecule showed once again independently that there are no individual electrons in a chemical bond, since the distance between them is less than the Compton wavelength.

When calculating, we assumed that the electrons move all the time along the chemical bond. Based on the mass defect and the values of real energies, we know for sure that the movement of electrons in a hydrogen molecule is more complex. Considering that the obtained distance between electrons is 92 times less than the Compton wavelength, it is quite obvious that exact calculations will also inevitably lead us to the region of the Compton wavelength.

And this means that the above physical justification of the chemical bond is correct and applicable to all chemical bonds (single-electron, two-electron, three-electron, etc.). It is simply necessary to clarify that in this consideration we represent the electron as a point particle.

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Note. “...The inertia of the particle in the direction of the velocity (longitudinal mass) is greater than perpendicular to the velocity (transverse mass)...

If the speed of a particle is close to the speed of light, then to change its speed in absolute value it is required to apply a much greater force than to change its direction. In other words, a very fast particle changes the direction of velocity more easily than its absolute value...” [4, p. 138].